# Exhibit 11

Kimberly Kaal, Environmental Manager, Shell Chemical Appalachia LLC, to Mark Gorog P.E., Regional Manager, Air Quality Program, DEP Southwest Regional Office, Re: PA-04-00740C Wastewater Treatment Plant (Source ID 502) Malodor and Excess Emissions Malfunction Report (Jan. 13, 2023) and Re: Malfunction Report as per PA-04-00740C Malodors from Wastewater Treatment Plant (WWTP) Shell Chemical Appalachia (Mar. 27, 2023).

Shell Chemical Appalachia LLC
300 Frankfort Rd
Monaca, PA 15061

January 13, 2023

Mark Gorog P.E., Regional Manager Air Quality Program
Pennsylvania Department of Environmental Protection Southwest Regional Office
400 Waterfront Drive
Pittsburgh, PA 15222

**RE: PA-04-00740C Wastewater Treatment Plant (Source ID 502) Malodor and Excess Emissions Malfunction Report**

Dear Mr. Gorog,

Shell Chemical Appalachia LLC ("Shell") is submitting this malfunction report to the Pennsylvania Department of Environmental Protection (PADEP) for odors and excess emissions from the wastewater treatment plant (WWTP)[1] between October 4 and December 13, 2022.

- **Name and location of the facility**
  Shell Polymers Monaca
  300 Frankfort Road, Monaca PA, 15061

- **Nature and cause of the incident**

  On November 6, 2022, Shell personnel detected a odor on site in the vicinity of the WWTP as part of regularly scheduled observations for potentially objectionable odors. Follow up offsite observational rounds by Shell's Emergency Response Team were initiated based upon the strength of the odor and judgement of observer. Shell personnel then detected faint similar odors during the offsite observations in the vicinity of Lockhouse 6 across the Ohio River. This offsite odor was considered to be malodor and reported to PADEP on the following business day.

  Odors had been observed within and around the WWTP on site prior to November 6 and increased observational rounds and area monitoring had already been implemented.[2] This included portable analyzer used to detect VOCs in the WWTP area, more frequent Operator and emergency response team observation rounds, as well as Shell maritime spill operator rounds near the shoreline to detect for odors. Water samples were taken from FEOR Tanks A and B on October 4, 2022 and form the basis for the beginning of the event emissions estimation. December 13, 2022 is the final day of any odors detected by Shell maritime spill operator at the river[3] and marks the

[1] WWTP including two biotreater aeration tanks.
[2] Odors had not been detected offsite by Shell prior to November 6 although olfactory rounds included onsite and offsite rounds.
[3] Contractor rounds were continued through the end of December without additional odor detection.

end of the event. Shell's contractor traveled up and down the river and did not find any other malodors.

Cause of the odors was determined to be the presence of accumulated hydrocarbons in the two biotreater aeration tanks of the WWTP coupled with ambient conditions which carried odors offsite and across the river. Hydrocarbons are received into the biotreater aeration tanks from the upstream flow equalization oil removal (FEOR) Tanks A and B. Source of the hydrocarbons into the FEOR Tanks was traced back to the ethane cracking unit (ECU) process wastewater. Incomplete separation of heavy hydrocarbons and water by the gasoline/water separator within the quench water system is the likely cause of elevated levels of heavy hydrocarbons entering the process wastewater stream from ECU.

Cause of the accumulation of hydrocarbons and biomaterial of top of the biotreaters was determined to be in part due to a misalignment of the skimmer rake, partially missing rubber skirt attached to the rake, and mistiming of the skimmer pump on Biotreater B. This degraded the ability of the skimmer system to remove accumulation from the top of the biotreaters for further processing the by the WWTP.

Corrective action and reduction of hydrocarbons from ECU has been implemented through improving souce control and separation of heavy hydrocarbons within ECU. An ECU wastewater sampling plan has been implemented along with target alarms to ensure streams are within design. This includes total organic carbon (TOC) correlations for ECU wastewater. A management of change project has been initiated for removal of waste oil/pitch from the quench water system in ECU and to limit heavier components from migrating downstream to WWTP.

Corrective action and mitigation of the accumulation of material on top of the biotreaters includes periodic vaccumming of the surface for disposal as a waste as well as utilizing capacity and hold times within each FEOR Tank to allow for additional removal time of hydrocarbons to recovered oil. Corrective action also includes periodic manual operation of the Biotreater B skimmer pump by Operations. Upstream improvements to source control (less hydrocarbons in the wastewater) have also reduced any accumulation and presence of odors. Replacement skimmer blades are on order and a plan to replace the rotating skimmer is in place. Additional assessment will be performed of the entire rotating assembly for any additional scope needed.

Additional long term corrective actions and process improvements are being evaluated or planned for implementation. Additional long term sampling and analysis of the FEOR Tanks is planned for updating modeling and long term emissions calculations.

- **Time when the incident was first observed, and duration of excess emissions**
  October 4, 2022 and intermittently until December 13, 2022. October 4 is the date of the FEOR Tank A and B water samples which forms the basis for inputs to the emissions model showing the air emissions from the biotreaters. As noted above, odors were not detected offsite by Shell between October 4 and November 6 although olfactory rounds included onsite and offsite rounds (See previous immediately above for duration of event clarification). December 13 is the final day that any odor was detected by the maritime spill operator along the river bank, which coincides with a period of 1 week of relatively lower stable TOC readings from FEOR Tank A and B samples.

- **Estimated rate of excess emissions**

Excess emissions for this malodor event have been calculated based upon an updated WATER9 Model, using FEOR Tank A and B water samples for speciated VOCs collected on October 4, using periodic FEOR Tank TOC sample results as indicators of elevated or low hydrocarbons, and measured flow rates into the biotreaters. The air emissions were modeled for what would have been emitted from the biotreaters. Sample results from each FEOR Tank contain volatile organics and HAPs including benzene, toluene, styrene, and naphthalene; with trace amounts of other HAPs present. All have been used as inputs to the updated model.

WATER9 Model outputs, inputs from sample results speciation, and inputs design parameters have been included as Attachment A.

| Pollutant | Emission Rate (tons) |
|---|---|
| VOC | 2.71 |
| HAP (Total) | 2.49 |
| Benzene | 2.01 |
| Toluene | 0.37 |
| Styrene | 0.05 |
| Naphthalene | 0.01 |

If you have any questions regarding this matter, please contact me at (724) 709-2467 or kimberly.kaal@shell.com.

Sincerely,

Kimberly Kaal

Kimberly Kaal
Environmental Manager, Attorney-in-Fact

CC:
Scott Beaudway, Air Quality Specialist
Anna Hensel, District Supervisor

**Attachment A**
**WATER9 Model Ouputs and Inputs**

**Table 1** **Air Emissions Calculations, Wastewater Treatment Plant, Water9 Output - Air Emissions, Malfunction Case**
**Shell Chemical Applachia LLC**

Air Emissions

| | Case 1: High Hydrocarbon Flow Case | | | | Case 2: Low Hydrocarbon Flow Case | | | | Total Malfunction Period |
|---|---|---|---|---|---|---|---|---|---|
| Component | Case 1 Emission Rate (g/s) | Case 1 Emission Rate (lb/hr) | Case 1 Emissions (lbs/ malfunction period) | Case 1 Emissions (tons/ malfunction period) | Case 2 Emission Rate (g/s) | Case 2 Emission Rate (lb/hr) | Case 2 Emissions (lbs/ malfunction period) | Case 2 Emissions (tons/ malfunction period) | Emissions (tons/ malfunction period) |
| Benzene | 7.05E-01 | 5.595 | 4,028.6 | 2.014 | 1.06E-02 | 0.084 | 82.8 | 0.041 | 2.056 |
| Phenol | 3.21E-08 | 0.000 | 0.0 | 0.000 | 3.46E-08 | 0.000 | 0.0 | 0.000 | 0.000 |
| Toluene | 1.22E-01 | 0.968 | 697.1 | 0.349 | 4.43E-03 | 0.035 | 34.6 | 0.017 | 0.366 |
| Ethylbenzene | 1.20E-03 | 0.010 | 6.9 | 0.003 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.003 |
| Xylene | 6.80E-04 | 0.005 | 3.9 | 0.002 | 8.85E-05 | 0.001 | 0.7 | 0.000 | 0.002 |
| Styrene | 1.67E-02 | 0.133 | 95.4 | 0.048 | 7.98E-04 | 0.006 | 6.2 | 0.003 | 0.051 |
| Naphthalene | 2.58E-03 | 0.020 | 14.7 | 0.007 | 2.49E-04 | 0.002 | 1.9 | 0.001 | 0.008 |
| 2 Methylnaphthalene | 7.09E-04 | 0.006 | 4.1 | 0.002 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.002 |
| Acenaphthene | 6.94E-05 | 0.001 | 0.4 | 0.000 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.000 |
| Acenaphthylene | 1.09E-04 | 0.001 | 0.6 | 0.000 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.000 |
| Fluorene | 4.99E-05 | 0.000 | 0.3 | 0.000 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.000 |
| Anthracene | 1.44E-05 | 0.000 | 0.1 | 0.000 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.000 |
| Phenanthrene | 4.77E-07 | 0.000 | 0.0 | 0.000 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.000 |
| Fluoranthene | 2.43E-07 | 0.000 | 0.0 | 0.000 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.000 |
| Pyrene | 8.05E-07 | 0.000 | 0.0 | 0.000 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.000 |
| Cyclopentadiene | 1.60E-03 | 0.013 | 9.1 | 0.005 | 1.73E-03 | 0.014 | 13.5 | 0.007 | 0.011 |
| Other Pentanes | 6.16E-03 | 0.049 | 35.2 | 0.018 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.018 |
| Other Hexanes | 1.02E-02 | 0.081 | 58.3 | 0.029 | 9.06E-03 | 0.072 | 70.8 | 0.035 | 0.065 |
| Other Heptanes | 5.18E-04 | 0.004 | 3.0 | 0.001 | 4.61E-04 | 0.004 | 3.6 | 0.002 | 0.003 |
| Other Octanes | 2.13E-03 | 0.017 | 12.2 | 0.006 | 2.13E-03 | 0.017 | 16.6 | 0.008 | 0.014 |
| Propyl (-n) Benzene | 1.96E-03 | 0.016 | 11.2 | 0.006 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.006 |
| 1,2,4-Trimethylbenzene | 6.22E-04 | 0.005 | 3.6 | 0.002 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.002 |
| Other Nonanes | 6.91E-03 | 0.055 | 39.5 | 0.020 | 3.00E-03 | 0.024 | 23.4 | 0.012 | 0.031 |
| 1,2,4,5 Tetramethylbenzene (1) | 6.17E-04 | 0.005 | 3.5 | 0.002 | 6.00E-04 | 0.005 | 4.7 | 0.002 | 0.004 |
| 1,2,4,5 Tetramethylbenzene (2) | 9.20E-04 | 0.007 | 5.3 | 0.003 | 9.95E-04 | 0.008 | 7.8 | 0.004 | 0.007 |
| Butyl Benzene | 5.87E-04 | 0.005 | 3.4 | 0.002 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.002 |
| Other Decanes+ | 8.64E-03 | 0.069 | 49.4 | 0.025 | 8.47E-03 | 0.067 | 66.1 | 0.033 | 0.058 |
| Total VOC | 8.90E-01 | 7.063 | 5,085.6 | 2.543 | 4.26E-02 | 0.338 | 332.8 | 0.166 | 2.709 |
| Total POM (excluding Naphthalene) | 9.53E-04 | 0.008 | 5.4 | 0.003 | 0.00E+00 | 0.000 | 0.0 | 0.000 | 0.003 |
| Total HAP | 8.49E-01 | 6.739 | 4,852.1 | 2.426 | 1.62E-02 | 0.128 | 126.2 | 0.063 | 2.489 |

Notes

1) Emission Rate (g/s) calculated in WATER9

2) Malfunction period was from 10/04/2022 to 12/13/2022, which is:

71 days

1704 hours

Malfunction period separated between 2 cases (High and Low Hydrocarbon Flows)

Case 1: High Hydrocarbon Flow Case: 30 days

720 hours

Case 2: Low Hydrocarbon Flow Case: 41 days

984 hours

**Table 2** **Air Emissions Calculations, Wastewater Treatment Plant, Water9 Composition Inputs, Malfunction Case**
**Shell Chemical Applachia LLC**

Sample Data - Input into Water9

| Component | Carbon Atoms | Component Molecular Weight (lb/lb-mol) | HAP? | POM? | FEOR-A - 16479 Concentration Sample Result (ug/L) | FEOR-A - 16479 Concentration Sample Result (mg/L) | FEOR-B - 16480 Concentration Sample Result (ug/L) | FEOR-B - 16480 Concentration Sample Result (mg/L) | Case 1: High Hydrocarbon Flow Case FEOR-T (input into Water9) Concentration (mg/L) | Case 2: DLow Hydrocarbon Flow Case FEOR-T (input into Water9) Concentration (mg/L) |
|---|---|---|---|---|---|---|---|---|---|---|
| Benzene | 6 | 78.11 | X | | 341.0 | 0.3410 | 299,000.0 | 299.0000 | 22.7404 | 0.3410 |
| Phenol | 6 | 94.11 | X | | 19.3 | 0.0193 | | 0.0000 | 0.0179 | 0.0193 |
| Toluene | 7 | 92.15 | X | | 187.0 | 0.1870 | 66,200.0 | 66.2000 | 5.1380 | 0.1870 |
| Ethylbenzene | 8 | 106.16 | X | | | 0.0000 | 608.0 | 0.6080 | 0.0456 | 0.0000 |
| Total Xylenes | 8 | 106.16 | X | | 6.9 | 0.0069 | 622.0 | 0.6220 | 0.0530 | 0.0069 |
| Styrene | 8 | 104.15 | X | | 15.6 | 0.0156 | 4,160.0 | 4.1600 | 0.3264 | 0.0156 |
| Naphthalene | 10 | 128.17 | X | X | 13.6 | 0.0136 | 1,710.0 | 1.7100 | 0.1408 | 0.0136 |
| 2-Methylnaphthalene | 11 | 142.2 | X | X | | 0.0000 | 197.0 | 0.1970 | 0.0148 | 0.0000 |
| Acenaphthene | 12 | 154.21 | X | X | | 0.0000 | 43.4 | 0.0434 | 0.0033 | 0.0000 |
| Acenaphthylene | 12 | 152.19 | X | X | | 0.0000 | 83.2 | 0.0832 | 0.0062 | 0.0000 |
| Fluorene | 13 | 166.22 | X | X | | 0.0000 | 51.5 | 0.0515 | 0.0039 | 0.0000 |
| Anthracene | 14 | 178.23 | X | X | | 0.0000 | 24.2 | 0.0242 | 0.0018 | 0.0000 |
| Phenanthrene | 14 | 178.23 | X | X | | 0.0000 | 81.3 | 0.0813 | 0.0061 | 0.0000 |
| Fluoranthene | 16 | 202.25 | X | X | | 0.0000 | 11.1 | 0.0111 | 0.0008 | 0.0000 |
| Pyrene | 16 | 202.25 | X | X | | 0.0000 | 22.1 | 0.0221 | 0.0017 | 0.0000 |
| 1,3-Cyclopentadiene | 5 | 66.1 | | | 30.1 | 0.0301 | | 0.0000 | 0.0278 | 0.0301 |
| * 1-Buten-3-yne, 2-methyl- | 5 | 66.1 | | | | 0.0000 | 1,420.0 | 1.4200 | 0.1065 | 0.0000 |
| * 1,3-Cyclopentadiene, 1-methyl- | 6 | 80.13 | | | 147.0 | 0.1470 | 246.0 | 0.2460 | 0.1544 | 0.1470 |
| * Ethylidenecyclobutane | 6 | 82.14 | | | 21.6 | 0.0216 | | 0.0000 | 0.0200 | 0.0216 |
| * Cyclobutane, ethenyl- | 6 | 82.14 | | | | 0.0000 | 200.0 | 0.2000 | 0.0150 | 0.0000 |
| * 1-Penten-3-yne, 2-methyl- | 6 | 80.13 | | | | 0.0000 | 10.5 | 0.0105 | 0.0008 | 0.0000 |
| * 1,4-Cyclohexadiene, 1-methy- | 7 | 94.15 | | | 8.4 | 0.0084 | | 0.0000 | 0.0077 | 0.0084 |
| * Bicyclo[2.2.1]hept-2-ene, 1-methyl | 7 | 94.15 | | | | 0.0000 | 18.0 | 0.0180 | 0.0014 | 0.0000 |
| * 3-Oxabicyclo[3.3.0]octan-2-one,6- | 8 | 138.16 | | | 13.5 | 0.0135 | | 0.0000 | 0.0125 | 0.0135 |
| * Bicyclo[2.2.1]hept-2-ene, 2-methyl | 8 | 108.18 | | | 24.9 | 0.0249 | | 0.0000 | 0.0230 | 0.0249 |
| * 9-Oxabicyclo[6.1.0]non-4-ene | 8 | 124.18 | | | | 0.0000 | 31.2 | 0.0312 | 0.0023 | 0.0000 |
| n-Propyl Benzene | 9 | 120.19 | | | | 0.0000 | 457.0 | 0.4570 | 0.0343 | 0.0000 |
| 1,2,4-Trimethylbenzene | 9 | 120.19 | | | | 0.0000 | 148.0 | 0.1480 | 0.0111 | 0.0000 |
| * 1H-Indene,3a,4,7,7a-tetrahydro | 9 | 120.19 | | | 12.8 | 0.0128 | 23.3 | 0.0233 | 0.0136 | 0.0128 |
| * Bicyclo[2.2.1]hept-2-ene, 5-ethenyl | 9 | 120.19 | | | 29.6 | 0.0296 | 901.0 | 0.9010 | 0.0950 | 0.0296 |
| * Indene | 9 | 116.16 | | | 9.3 | 0.0093 | 21.3 | 0.0213 | 0.0102 | 0.0093 |
| * Tricyclo[3.3.0.0(2,8)]octan-3-one | 9 | 136.19 | | | | 0.0000 | 19.5 | 0.0195 | 0.0015 | 0.0000 |
| Benzene, 1,2,4,5-tetramethyl-(01) | 10 | 134.22 | | | 10.5 | 0.0105 | 14.4 | 0.0144 | 0.0108 | 0.0105 |
| Benzene, 1,2,4,5-tetramethyl-(02) | 10 | 134.22 | | | 17.4 | 0.0174 | | 0.0000 | 0.0161 | 0.0174 |
| Butylbenzene | 10 | 134.22 | | | | 0.0000 | 139.0 | 0.1390 | 0.0104 | 0.0000 |
| * Benzene, 2-ethyl-1,4-dimethyl- | 10 | 134.22 | | | 10.8 | 0.0108 | 14.4 | 0.0144 | 0.0111 | 0.0108 |
| * 2,4-Dimethylstyrene | 10 | 132.2 | | | 8.5 | 0.0085 | | 0.0000 | 0.0079 | 0.0085 |
| * Benzene,1,3-diethyl- | 10 | 134.22 | | | 23.2 | 0.0232 | | 0.0000 | 0.0215 | 0.0232 |
| * Benzene,1-methyl-3-propyl- | 10 | 134.22 | | | 13.7 | 0.0137 | | 0.0000 | 0.0127 | 0.0137 |
| * cis-8-Methyl-bicyclo(4,3,0)non-3,7 | 10 | 134.22 | | | 49.1 | 0.0491 | 64.5 | 0.0645 | 0.0503 | 0.0491 |
| * Benzene, 1-methyl-3-(1-methylethyl)- | 10 | 134.22 | | | 9.5 | 0.0095 | 12.9 | 0.0129 | 0.0097 | 0.0095 |
| * 1,4,4a,5,8,8a-Hexahydro-naphthalen | 10 | 134.22 | | | 13.2 | 0.0132 | 21.4 | 0.0214 | 0.0138 | 0.0132 |
| * Benzene,1-methyl-2-propyl- | 10 | 134.22 | | | | 0.0000 | 19.1 | 0.0191 | 0.0014 | 0.0000 |
| * 1-Phenyl-1-butene | 10 | 132.2 | | | | 0.0000 | 11.8 | 0.0118 | 0.0009 | 0.0000 |
| * Benzene, 1,2,3,5-tetramethyl- | 10 | 134.22 | | | | 0.0000 | 22.6 | 0.0226 | 0.0017 | 0.0000 |
| * Benzene, pentamethyl- | 11 | 148.24 | | | 7.3 | 0.0073 | | 0.0000 | 0.0067 | 0.0073 |
| * 5-Phenylbicyclo[2.2.1]hept-2-ene | 13 | 170.25 | | | 12.0 | 0.0120 | 13.1 | 0.0131 | 0.0121 | 0.0120 |

Notes

1) FEOR-A and FEOR-B samples from Environmental Service Laboratories, INC. lab results from 10/04/2022 sample

2) If daily TOC reading is ≥ 84.76 mg/l, FEOR-T is calculated assuming the following contributions from FEOR-A and FEOR-B:

| | | |
|---|---|---|
| FEOR-A | 92.5 | % contribution to FEOR-T |
| FEOR-B | 7.5 | % contribution to FEOR-T |

This assumption is based off of: Wastewater is fed to the biotreater from one FEOR at a time, and high hydrocarbon flow will trickle in from the other FEOR. A conservative case is 5-10% of high hydrocarbon FEOR to be trickled in, therefore, an average of the high hydrocarbon FEOR of 7.5% will be used for the spilt of FEOR A/B.

3) If daily TOC reading is < 84.76 mg/l, FEOR-T is assumed 100% FEOR-A. See 'Input_FEOR_A_B_T' tab for backup.

4) A subset of components above were not available within the Water9 database (desginated with an *), so they were grouped by carbon atoms and input into Water9 according to:

| Component | Case 1 Concentration (mg/L) | Case 2 Concentration (mg/L) |
|---|---|---|
| Pentanes | 0.107 | 0.000 |
| Hexanes | 0.190 | 0.169 |
| Heptanes | 0.009 | 0.008 |
| Octanes | 0.038 | 0.038 |
| Nonanes | 0.120 | 0.052 |
| Decanes+ | 0.150 | 0.147 |

Note: for Hexanes, n-Hexane is only surrogate available in Water9, so it was chosen for the model, but n-Hexane is not present and will be treated as 'Other Hexanes'

**Table 3** **Air Emissions Calculations, Wastewater Treatment Plant, Water9 Data Inputs, Malfunction Case**
**Shell Chemical Applachia LLC**

Waste Stream Input Assumptions

| Water9 Parameter | FEOR-T | CT-BLOW |
|---|---|---|
| Flow (l/s) | 57.6 | 89 |
| Solids (ppm) | 162 | 20 |
| Oil (ppm) | 24 | |
| Dis Sol (ppm) | 5,000 | 1,896 |
| Temp (F) | 41 | 42 |

Waste Set Inputs assumed from the company supplied data: *Marked_Air_Plan_Approval.pdf*
FEOR-T Flow - See 'Input_FEOR_A_B_T' tab for backup

Wastewater Treatment Plant Unit Inputs into Water9

Unit Inputs assumed from the company supplied data: *Marked_Air_Plan_Approval.pdf*

| Diffused air biotreatment | Water9 input | Water9 input |
|---|---|---|
| 1 Description of unit | Diffused air bio - unit 28 | Diffused air bio - unit 29 |
| 2 Wastewater temperature ( C) | 25 | 25 |
| 3 length of aeration unit (m) | 26.7 | 26.7 |
| 4 width of aeration unit (m) | 26.7 | 26.7 |
| 5 depth of aeration unit (m) | 7.9 | 7.9 |
| 6 fraction of surface agitated by air | 0.8 | 0.8 |
| 7 fraction of surface quiescent | 0.2 | 0.2 |
| 13 if there is plug flow, enter 1 | 0 | 0 |
| 14 Overall biorate (mg/g bio-hr) | 19 | 19 |
| 15 Aeration air flow (m3/s) | 1.711 | 1.711 |
| 16 activated sludge biomass (g/l) | 2 | 2 |
| 17 If covered, then enter 1 | 0 | 0 |
| 18 special input | 0 | 0 |
| 19 pH (enter 0 for no pH adjustment) | 0 | 0 |

| Circular clarifiers | Water9 input | Water9 input |
|---|---|---|
| 1 Description of unit | Clarifier 1 - unit 2 | Clarifier 2 - unit 7 |
| 2 Wastewater temperature ( C) | 25 | 25 |
| 3 secondary clarifier diameter (m) | 19.3 | 19.3 |
| 4 secondary clarifier depth (m) | 5.6 | 5.6 |
| 5 clarifier solids removal efficiency | 0.7 | 0.7 |
| 6 waterfall drop height (cm) | 20 | 20 |
| 7 clarifier weir/circumference | 0.5 | 0.5 |
| 8 Center well present, =1 | 0 | 0 |
| 10 number of identical units in parallel | 1 | 1 |
| 19 pH (enter 0 for no pH adjustment) | 0 | 0 |

| Open sump | Water9 input |
|---|---|
| 1 Description of unit | Biosluge sump - unit 16 |
| 2 Underflow T ( C) | 25 |
| 3 Total water added at the unit (l/s) | 0 |
| 4 Area of openings at unit (cm2) | 50 |
| 5 Radius of drop pipe (cm) | 5 |
| 6 Drop length to conduit (cm) | 61 |
| 7 Open surface=1 | 1 |
| 8 Subsurface entrance=1 | 0 |
| 9 subsurface exit =1 | 0 |
| 10 radius of underflow conduit (cm | 12 |
| 11 distance to next unit (cm) | 500 |
| 12 slope of underflow conduit | 0.015 |
| 13 Open surface of liquid at the unit (cm2) | 90000 |
| 14 flow entrance depth under surface | 10 |
| 15 depth of liquid in sump (cm) | 168 |

| | |
|---|---|
| 16 velocity air at opening (ft/min) | 88 |
| 17 municipal waste in conduit =1 | 0 |
| 18 Assume equilibrium in unit, =1 | 0 |
| 19 pH (enter 0 for no pH adjustment) | 0 |

| **Storage tank** | **Water9 input** | **Water9 input** |
|---|---|---|
| 1 Description of unit | Biosluge holding - unit 13 | Biosludge tank - unit 12 |
| 2 Wastewater temperature ( C) | 25 | 42 |
| 3 Open surface area of tank (m2) | 16.6 | 34.2 |
| 4 Density of liquid in tank (g/cc) | 1 | 1 |
| 5 tank wast Mwt, water=18 | 18 | 18 |
| 6 unit storage time (days) | 0 | 0 |
| 7 tank paint factor | 0.6 | 0.6 |
| 8 tank diameter | 4.6 | 6.6 |
| 9 tank vapor space height (m) | 0.64 | 1.1 |
| 10 diurnal tamp. Change (deg. C) | 11 | 11 |
| 11 tank height (m) | 3.2 | 5.5 |
| 12 oil in composite wastewater (Wt. %) | 0 | 0 |
| 13 Product factor crude oil =0.75 else 1.0 | 1 | 1 |
| 19 pH (enter 0 for no pH adjustment) | 0 | 0 |

| **DAF or grit separator** | **Water9 input** |
|---|---|
| 1 Description of unit | Sand Filter - unit 30 |
| 2 Wastewater temperature ( C) | 42 |
| 3 KL unit surface (m/s) | 0.001 |
| 4 Pretreatment length (m) | 3.6 |
| 5 Pretreatment width (m) | 2.7 |
| 6 Pretreatment depth (m) | 3 |
| 7 air flow (m3/s) | 0.193 |
| 8 oil in composite wastewater (Wt. %) | 0 |
| 9 fraction surface covered with float | 0 |
| 10 Oil molecular weight | 180 |
| 11 Density of oil (g/cc) | 1 |
| 12 active biomass, (g/l) | 0 |
| 13 number units in parallel | 0 |
| 15 vent air emission control factor | 0 |
| 16 cover vent rate (m3/s per m2 surface) | 0.02 |
| 17 If covered, then enter 1 | 1 |
| 19 pH (enter 0 for no pH adjustment) | 0 |

| **Weir, waterfall** | **Water9 input** |
|---|---|
| 1 Description of unit | Outfall - unit 9 |
| 2 Underflow T ( C) | 42 |
| 3 Total water added at the unit (l/s) | 0 |
| 4 waterfall width at surface (m) | 3 |
| 5 waterfall drop height (cm) | 20 |
| 6 tailwater depth (m) | 0.1 |
| 7 Open surface=1 | 1 |
| 8 Subsurface entrance=1 | 1 |
| 9 subsurface exit =1 | 0 |
| 10 radius of underflow conduit (cm) | 12 |
| 11 distance to next unit (cm) | 500 |
| 12 slope of underflow conduit | 0.015 |
| 19 pH (enter 0 for no pH adjustment) | 0 |

Shell Chemical Appalachia LLC
300 Frankfort Rd
Monaca, PA 15061

March 27, 2023

Mark Gorog P.E., Regional Manager Air Quality Program
Pennsylvania Department of Environmental Protection (PADEP)
Southwest Regional Office
400 Waterfront Drive
Pittsburgh, PA 15222

**RE: Malfunction Report as per PA-04-00740C**
**Malodors fromWastewater Treatment Plant (WWTP)**
**Shell Chemical Appalachia LLC**

Dear Mr. Gorog,

Shell Chemical Appalachia LLC ("Shell") is submitting this Malfunction Report to the Pennsylvania Department of Environmental Protection (PADEP) for malodors detectable outside the property from the waste water treatment plant (WWTP) (Source ID 502). The format of this and future malfunction reports has been updated as requested by PADEP.

This malfunction did not pose danger to the public health and safety or the environment. Shell personnel detected faint similar odors during the offsite observations in the vicinity of Gate 3 and Lockhouse 6 across the Ohio River. This offsite odor was considered to be malodor and reported to PADEP. Shell's third-party contractor conducted offsite odor surveys and hydrocarbon sampling encompassing Route 18 west to Raccoon Creek and east to Beaver Valley Mall area, 376 south to Route 18 and North to Vanport area, and Route 68 west to Lockhouse 6 restaurant and east to Vanport and Beaver areas.

- **Name and location of the facility**
  Shell Polymers Monaca
  300 Frankfort Road, Monaca PA, 15061

- **Nature and cause of the malfunction or breakdown**
  Malodors were detected outside the property. Cause of the odors was hydrocarbons in the WWTP biotreaters.

- **Time when the malfunction or breakdown was first observed**
  January 25, 2023 at ~09:45AM when a malodor was first detected offsite.

- **The date and time that the malfunction started and ended**
  January 25, 2023 beginning at 09:45AM and ending on February 16, 2023 at ~1:58PM when a malodor was last detected offsite.

- **An estimate of the emissions associated with the malfunction**

*Table 1: Preliminary total estimated excess emissions onsite for the biotreater*

| Pollutant | Emission Rate (tons) |
|---|---|
| VOC | 0.46 |
| HAP (Total) | 0.41 |
| Benzene | 0.26 |
| Toluene | 0.13 |

- **The calculations that were used to determine that quantity**

Excess emissions for this malodor event have been calculated using the Environmental Protection Agency's (EPA) updated WATER9 Model, using periodic wastewater sample results for volatile organics and semi-volatile organics taken at the biotreater inlet and flow equalization and oil removal tanks, application of process indicators and operating condition wastewater retention times, and measured flow rates into the biotreaters. Sample results contain volatile organics and Hazardous Air Pollutants (HAPs) including benzene, and toluene; with trace amounts of other HAPs present. All have been used as inputs to the updated model.

WATER9 Model outputs, inputs from sample results speciation, and inputs design parameters have been included as Attachment A

- **The steps, if any, that the facility took to limit the duration and/or quantity of emissions associated with the malfunction**

Odors were minimized through operational control of flow equilization and oil recovery (FEOR) tank B to receive wastewater which may contain higher levels of hydrocarbons when possible and FEOR A retained wastewater containing lower levels of hydrocarbons. Hydrocarbon-containing wastewater was integrated slowly when possible from FEOR B into the combined flow entering the biotreaters. This minimized hydrocarbons in the biotreaters, allowed time for biodegradation of organic material, and limited hydrocarbon levels that could generate odors.

Odors were minimized through added process wastewater sampling within the ethane cracking unit (ECU) to determine when process wastewater conditions improved or worsened and enabling communication to the WWTP for better wastewater flow management. This sampling also contributed to root cause determination and corrective actions.

Odors were minimized through the closure of a manual valve and isolating the ECU wash oil slop drum, hydrocarbon slop drum, and warm flare drum liquids from the process wastewater system. Operations walked down the piping and hydrocarbon-containing drums within ECU to verify line-ups for pumping. This reduced hydrocarbons entering the wastewater by enabling the pumping and recycling of hydrocarbons back into the closed-loop process.

- **A detailed analysis that sets forth the Root Cause of the malfunction, to the extent determinable**

The root cause of offsite detectable odors was determined to be hydrocarbons coming from the ECU leading to the WWTP. The valve was opened in response to an abnormal process condition but was not returned to its normal closed state. This caused pumping of hydrocarbons from the affected drums to be sent to the WWTP for longer than intended instead of recycling back into the process. This led to higher levels of hydrocarbons entering the biotreaters periodically and generating odors. Normal operation is hydrocarbon-containing drums are either recycled back into the process and separated and sent to storage as a byproduct, or loaded out as a waste.

- **An analysis of the measures, if any, that are available to reduce the likelihood of a**

**recurrence of a malfunction resulting from the same Root Cause or contributing causes in the future**

A management of change was initiated to evaluate and install a car-seal on the manual valve VA-190172-2 isolating the process wastewater from the hydrocarbon-containing drums within ECU. Car-sealing this manual valve closed provides a higher level of control and assurance on the valve operation. Line labeleing has also been added to this piping manifold to clearly identify process streams, and approval and notification necessary for valve operation. Car-seals have been added to other valves within ECU to similarly provide a higher level of control against contamination between other process streams that could lead to equipment damage or other malfunctions.

Shell commissioned a project to design and install a temporary enclosed induced air flotation system to improve and increase hydrocarbon removal capacity in the WWTP. Separated hydrocarbons will be routed to the recovered oil tank and overhead vapors from the enclosed system routed to the spent caustic thermal oxidizer consistent with the original design intent of the WWTP. Approval has been received from the PADEP Water Quality Program for this temporary installation and has been requested from the Air Quality Program through the Request for Determination process. Odors in the future will be minimized by the reduction of hydrocarbons entering the biotreaters and destruction of vapors in the thermal oxidizer. Offsite odor detections have ended prior to implementation of this project but the action began during the event. Performance of this temporary project will be evaluated for potential design of a similar permanent system.

- **To the extent that investigations of the causes and/or possible corrective action(s) still are underway on the due date of the report, a statement of the anticipated date by which a follow-up report will be submitted**

  No follow up report planned. A follow up request for determination or application will be sent as necessary based on PADEP's response to the induced air flotation temporary project.

- **Corrective action is final or timeline for implementation**

  Corrective action to eliminate malodors detectable offsite is considered final. Installation and evaluation of a temporary enclosed diffused air flotation in the WWTP is expected to be commenced in the next month.

If you have any questions regarding this matter, please contact me at (724) 709-2467 or kimberly.kaal@shell.com.

Sincerely,

Kimberly J. Kaal

Kimberly Kaal
Environmental Manager, Attorney-in-Fact

CC:
Scott Beaudway, Air Quality Specialist
Beth Speicher, Environmental Group Manager

**Attachment A**
**WATER9 Model Ouputs and Inputs**

**Wastewater Treatment Plant, Malfunction Emissions**
**Shell Polymers Monaca**

Incident Start Time: 1/25/2023
Incident End Time: 2/16/2023

| Timeline Run Start Date | Timeline Run End Date | Timeline Run Number of Days | FEOR- T Flowrate (l/sec) | Sample Date/Location | Malfunction Start Date | Malfunction Start Date | Malfunction Number of Days | % of Emissions Based on Days | Total VOC Emissions (tons) | Total HAP Emissions (tons) | Benzene Emissions (tons) | Phenol Emissions (tons) | Toluene Emissions (tons) | Ethylbenzene Emissions (tons) | Xylene Emissions (tons) | Styrene Emissions (tons) | Naphthalene Emissions (tons) | POM (minus naphthalene) Emissions (tons) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1/15/2023 | 2/8/2023 | 24.625 | 63.3 | 10/4/2022 FEOR A | 1/25/2023 | 2/8/2023 | 15 | 60.9137 | 0.0701 | 0.0281 | 0.0183 | 0.0000 | 0.0079 | 0.0000 | 0.0002 | 0.0013 | 0.0005 | 0.0000 |
| 1/15/2023 | 2/8/2023 | 0.375 | 7.0 | 1/10/2023 FEOR B | 1/25/2023 | 2/8/2023 | 0.375 | 100.0000 | 0.0032 | 0.0032 | 0.0019 | 0.0000 | 0.0010 | 0.0000 | 0.0000 | 0.0001 | 0.0002 | 0.0000 |
| 2/9/2023 | 2/9/2023 | 0.5 | 69.4 | 2/9/2023 Biotreater Inlet | 2/9/2023 | 2/9/2023 | 0.5 | 100.0000 | 0.2488 | 0.2488 | 0.1548 | 0.0000 | 0.0762 | 0.0063 | 0.0000 | 0.0111 | 0.0005 | 0.0000 |
| 2/9/2023 | 2/10/2023 | 1.5 | 67.6 | 2/9/2023 Biotreater Inlet; diluted by 6.5 | 2/9/2023 | 2/10/2023 | 1.5 | 100.0000 | 0.1059 | 0.1059 | 0.0689 | 0.0000 | 0.0340 | 0.0028 | 0.0000 | 0.0000 | 0.0002 | 0.0000 |
| 2/11/2023 | 2/11/2023 | 1 | 61.5 | 2/9/2023 Biotreater Inlet; diluted by 6.5, then another 6.5 | 2/11/2023 | 2/11/2023 | 1 | 100.0000 | 0.0099 | 0.0099 | 0.0064 | 0.0000 | 0.0032 | 0.0003 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 2/12/2023 | 2/20/2023 | 8.875 | 58.0 | 10/4/2022 FEOR A | 2/12/2023 | 2/16/2023 | 5 | 56.3380 | 0.0214 | 0.0086 | 0.0056 | 0.0000 | 0.0024 | 0.0000 | 0.0001 | 0.0004 | 0.0001 | 0.0000 |
| 2/12/2023 | 2/20/2023 | 0.125 | 6.4 | 1/10/2023 FEOR B | 2/12/2023 | 2/16/2023 | 0.125 | 100.0000 | 0.0010 | 0.0010 | 0.0006 | 0.0000 | 0.0003 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| | | | | | | | | | 0.4602 | 0.4054 | 0.2564 | 0.0000 | 0.1250 | 0.0094 | 0.0002 | 0.0129 | 0.0015 | 0.0001 |

**Wastewater Treatment Plant, Water9 Emission Inputs**
**Shell Polymers Monaca**

Data Sources

Marked_Air_Plan_Approval.pdf - plan approval assumptions vetted by Operations.
3/13/2023 email Process Engineering for the Biotreater agitated/quiescent fractions

Waste Stream Input Assumptions

| Water9 Parameter | FEOR-T | CT-BLOW |
|---|---|---|
| Solids (ppm) | 162 | 20 |
| Oil (ppm) | 24 | |
| Dissolved Solids (ppm) | 5,000 | 1,896 |
| Temp (C) | 25 | 25 |

Wastewater Treatment Plant Unit Inputs into Water9

| Diffused air biotreatment | Water9 input | Water9 input |
|---|---|---|
| 1 Description of unit | Diffused air bio - unit 28 | Diffused air bio - unit 29 |
| 2 Wastewater temperature ( C) | 25 | 25 |
| 3 length of aeration unit (m) | 24.8 | 24.8 |
| 4 width of aeration unit (m) | 24.8 | 24.8 |
| 5 depth of aeration unit (m) | 6.1 | 6.1 |
| 6 fraction of surface agitated by air | 0.72 | 0.72 |
| 7 fraction of surface quiescent | 0.28 | 0.28 |
| 13 if there is plug flow, enter 1 | 0 | 0 |
| 14 Overall biorate (mg/g bio-hr) | 19 | 19 |
| 15 Aeration air flow (m3/s) | 1.711 | 1.711 |
| 16 activated sludge biomass (g/l) | 2 | 2 |
| 17 If covered, then enter 1 | 0 | 0 |
| 18 special input | 0 | 0 |
| 19 pH (enter 0 for no pH adjustment) | 0 | 0 |

| Circular clarifiers | Water9 input | Water9 input |
|---|---|---|
| 1 Description of unit | Clarifier 1 - unit 2 | Clarifier 2 - unit 7 |
| 2 Wastewater temperature ( C) | 25 | 25 |
| 3 secondary clarifier diameter (m) | 17.2 | 17.2 |
| 4 secondary clarifier depth (m) | 6.1 | 6.1 |
| 5 clarifier solids removal efficiency | 0.7 | 0.7 |
| 6 waterfall drop height (cm) | 20 | 20 |
| 7 clarifier weir/circumference | 0.5 | 0.5 |
| 8 Center well present, =1 | 0 | 0 |
| 10 number of identical units in parallel | 1 | 1 |
| 19 pH (enter 0 for no pH adjustment) | 0 | 0 |

| Open sump | Water9 input |
|---|---|
| 1 Description of unit | Biosluge sump - unit 16 |
| 2 Underflow T ( C) | 25 |
| 3 Total water added at the unit (l/s) | 0 |
| 4 Area of openings at unit (cm2) | 50 |
| 5 Radius of drop pipe (cm) | 5 |
| 6 Drop length to conduit (cm) | 61 |
| 7 Open surface=1 | 1 |
| 8 Subsurface entrance=1 | 0 |
| 9 subsurface exit =1 | 0 |
| 10 radius of underflow conduit (cm | 12 |
| 11 distance to next unit (cm) | 500 |
| 12 slope of underflow conduit | 0.015 |
| 13 Open surface of liquid at the unit (cm2) | 90000 |
| 14 flow entrance depth under surface | 10 |
| 15 depth of liquid in sump (cm) | 168 |
| 16 velocity air at opening (ft/min) | 88 |
| 17 municipal waste in conduit =1 | 0 |
| 18 Assume equilibrium in unit, =1 | 0 |
| 19 pH (enter 0 for no pH adjustment) | 0 |

| Storage tank | Water9 input | Water9 input |
|---|---|---|
| | Biosluge holding - unit 13 | Biosludge tank - unit 12 |
| 2 Wastewater temperature ( C) | 25 | 42 |
| 3 Open surface area of tank (m2) | 16.6 | 34.2 |
| 4 Density of liquid in tank (g/cc) | 1 | 1 |
| 5 tank wast Mwt, water=18 | 18 | 18 |
| 6 unit storage time (days) | 0 | 0 |
| 7 tank paint factor | 0.6 | 0.6 |
| 8 tank diameter | 4.6 | 6.6 |
| 9 tank vapor space height (m) | 0.64 | 1.1 |
| 10 diurnal tamp. Change (deg. C) | 11 | 11 |
| 11 tank height (m) | 3.2 | 5.5 |
| 12 oil in composite wastewater (Wt. %) | 0 | 0 |
| 13 Product factor crude oil =0.75 else 1.0 | 1 | 1 |
| 19 pH (enter 0 for no pH adjustment) | 0 | 0 |

| DAF or grit separator | Water9 input |
|---|---|
| 1 Description of unit | Sand Filter - unit 30 |
| 2 Wastewater temperature ( C) | 42 |
| 3 KL unit surface (m/s) | 0.001 |
| 4 Pretreatment length (m) | 3.6 |
| 5 Pretreatment width (m) | 2.7 |
| 6 Pretreatment depth (m) | 3 |
| 7 air flow (m3/s) | 0.193 |
| 8 oil in composite wastewater (Wt. %) | 0 |
| 9 fraction surface covered with float | 0 |
| 10 Oil molecular weight | 180 |
| 11 Density of oil (g/cc) | 1 |
| 12 active biomass, (g/l) | 0 |
| 13 number units in parallel | 0 |
| 15 vent air emission control factor | 0 |
| 16 cover vent rate (m3/s per m2 surface) | 0.02 |
| 17 If covered, then enter 1 | 1 |
| 19 pH (enter 0 for no pH adjustment) | 0 |

| Weir, waterfall | Water9 input |
|---|---|
| 1 Description of unit | Outfall - unit 9 |
| 2 Underflow T ( C) | 42 |
| 3 Total water added at the unit (l/s) | 0 |
| 4 waterfall width at surface (m) | 3 |
| 5 waterfall drop height (cm) | 20 |
| 6 tailwater depth (m) | 0.1 |
| 7 Open surface=1 | 1 |
| 8 Subsurface entrance=1 | 1 |
| 9 subsurface exit =1 | 0 |
| 10 radius of underflow conduit (cm) | 12 |
| 11 distance to next unit (cm) | 500 |
| 12 slope of underflow conduit | 0.015 |
| 19 pH (enter 0 for no pH adjustment) | 0 |

**Wastewater Treatment Plant, Summary of Analytical Data**
**Shell Polymers Monaca**

| Sample Date | | | | | 10/4/2022 | 1/10/2023 | 2/9/2023 | 2/9/2023 | 2/9/2023 |
|---|---|---|---|---|---|---|---|---|---|
| Sample Time | | | | | 9:50 | 14:00 | 12:00 | 12:00 | 12:00 |
| Sample ID | | | | | 16479 | 29034 | 180-15833-1 | 180-15833-1 | 180-15833-1 |
| Sample Location | | | | | FEOR A | FEOR B | Biotreater Inlet | Biotreater Inlet; diluted by 6.5 | Biotreater Inlet; diluted by 6.5, then another 6.5 |
| Analytical Method | | | | | EPA 624/625 | EPA 624.1/625.1 | EPA 624.1/625.1 | EPA 624.1/625.1 | EPA 624.1/625.1 |
| Lab | | | | | ESL | Eurofins | Eurofins | Eurofins | Eurofins |
| Component | Carbon Atoms | Component Molecular Weight (lb/lb-mol) | HAP? | POM? | Concentration Sample Result (mg/L) | Concentration Sample Result (mg/L) | Concentration Sample Result (mg/L) | Concentration Sample Result (mg/L) | Concentration Sample Result (mg/L) |
| Benzene | 6 | 78.11 | X | | 0.3410 | 13.0000 | 78.0000 | 12.0000 | 1.8462 |
| Phenol | 6 | 94.11 | X | | 0.0193 | | | | |
| Toluene | 7 | 92.15 | X | | 0.1870 | 8.3000 | 49.0000 | 7.5385 | 1.1598 |
| Ethylbenzene | 8 | 106.16 | X | | | | 3.7000 | 0.5692 | 0.0876 |
| Total Xylenes | 8 | 106.16 | X | | 0.0069 | | | | |
| Styrene | 8 | 104.15 | X | | 0.0156 | 0.4100 | 3.7000 | | |
| Naphthalene | 10 | 128.17 | X | X | 0.0136 | 1.6000 | 0.3900 | 0.0600 | 0.0092 |
| 2-Methylnaphthalene | 11 | 142.2 | X | X | | | | | |
| Acenaphthene | 12 | 154.21 | X | X | | 0.0770 | 0.0059 | 0.0009 | 0.0001 |
| Acenaphthylene | 12 | 152.19 | X | X | | 0.0480 | 0.0019 | 0.0003 | 0.0000 |
| Fluorene | 13 | 166.22 | X | X | | 0.0900 | 0.0032 | 0.0005 | 0.0001 |
| Anthracene | 14 | 178.23 | X | X | | 0.0110 | 0.0005 | 0.0001 | 0.0000 |
| Phenanthrene | 14 | 178.23 | X | X | | 0.0980 | 0.0037 | 0.0006 | 0.0001 |
| Fluoranthene | 16 | 202.25 | X | X | | 0.0110 | 0.0007 | 0.0001 | 0.0000 |
| Pyrene | 16 | 202.25 | X | X | | 0.0130 | 0.0009 | 0.0001 | 0.0000 |
| Benzo(a)anthracene | 18 | 228.29 | X | X | | 0.0014 | | | |
| Chrysene | 18 | 228.29 | X | X | | 0.0013 | | | |
| 1,3-Cyclopentadiene | 5 | 66.1 | | | 0.0301 | | | | |
| * 1-Buten-3-yne, 2-methyl- | 5 | 66.1 | | | | | | | |
| * 1,3-Cyclopentadiene, 1-methyl- | 6 | 80.13 | | | 0.1470 | | | | |
| * Ethylidenecyclobutane | 6 | 82.14 | | | 0.0216 | | | | |
| * Cyclobutane, ethenyl- | 6 | 82.14 | | | | | | | |
| * 1-Penten-3-yne, 2-methyl- | 6 | 80.13 | | | | | | | |
| * 1,4-Cyclohexadiene, 1-methy- | 7 | 94.15 | | | 0.0084 | | | | |
| * Bicyclo[2.2.1]hept-2-ene, 1-methyl | 7 | 94.15 | | | | | | | |
| * 3-Oxabicyclo[3.3.0]octan-2-one,6- | 8 | 138.16 | | | 0.0135 | | | | |
| * Bicyclo[2.2.1]hept-2-ene, 2-methyl | 8 | 108.18 | | | 0.0249 | | | | |
| * 9-Oxabicyclo[6.1.0]non-4-ene | 8 | 124.18 | | | | | | | |
| n-Propyl Benzene | 9 | 120.19 | | | | | | | |
| 1,2,4-Trimethylbenzene | 9 | 120.19 | | | | | | | |
| * 1H-Indene,3a,4,7,7a-tetrahydro | 9 | 120.19 | | | 0.0128 | | | | |
| * Bicyclo[2.2.1]hept-2-ene, 5-ethenyl | 9 | 120.19 | | | 0.0296 | | | | |
| * Indene | 9 | 116.16 | | | 0.0093 | | | | |
| * Tricyclo[3.3.0.0(2,8)]octan-3-one | 9 | 136.19 | | | | | | | |
| Benzene, 1,2,4,5-tetramethyl-(01) | 10 | 134.22 | | | 0.0105 | | | | |
| Benzene, 1,2,4,5-tetramethyl-(02) | 10 | 134.22 | | | 0.0174 | | | | |
| Butylbenzene | 10 | 134.22 | | | | | | | |
| * Benzene, 2-ethyl-1,4-dimethyl- | 10 | 134.22 | | | 0.0108 | | | | |
| * 2,4-Dimethylstyrene | 10 | 132.2 | | | 0.0085 | | | | |
| * Benzene,1,3-diethyl- | 10 | 134.22 | | | 0.0232 | | | | |
| * Benzene,1-methyl-3-propyl- | 10 | 134.22 | | | 0.0137 | | | | |
| * cis-8-Methyl-bicyclo(4,3,0)non-3,7 | 10 | 134.22 | | | 0.0491 | | | | |
| * Benzene, 1-methyl-3-(1-methylethyl)- | 10 | 134.22 | | | 0.0095 | | | | |
| * 1,4,4a,5,8,8a-Hexahydro-naphthalen | 10 | 134.22 | | | 0.0132 | | | | |
| * Benzene,1-methyl-2-propyl- | 10 | 134.22 | | | | | | | |
| * 1-Phenyl-1-butene | 10 | 132.2 | | | | | | | |
| * Benzene, 1,2,3,5-tetramethyl- | 10 | 134.22 | | | | | | | |
| * Benzene, pentamethyl- | 11 | 148.24 | | | 0.0073 | | | | |
| * 5-Phenylbicyclo[2.2.1]hept-2-ene | 13 | 170.25 | | | 0.0120 | | | | |
| Pentanes | 5 | | | | 0 | | | | |
| Hexanes | 6 | | | | 0.1686 | | | | |
| Heptanes | 7 | | | | 0.0084 | | | | |
| Octanes | 8 | | | | 0.0384 | | | | |
| Nonanes | 9 | | | | 0.0517 | | | | |
| Decanes + | 10+ | | | | 0.1473 | | | | |

*A subset of components above were not available within the Water9 database (desginated with an *), so they were grouped by carbon atoms and input into Water9 as Pentanes, Hexanes, Heptanes, Octanes, Nonanes and Decanes.
Note: for Hexanes, n-Hexane is only surrogate available in Water9, so it was chosen for the model, but n-Hexane is not present and will be treated as 'Other Hexanes